Nuclear Modeling for Cross Sections

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Science Modeling & Computation for AFCI

Impact

- Long term: New developments in modeling and simulation will have biggest impact on fast reactors in long-range time scale (> 20 years)

- Short-term: Ongoing work on nuclear data, materials modeling and separations science, especially when expanded, can have significant impact in the short term (5 to 10 years)

Critical needs

- Methods to deal with multi-scale physics in terms of different models and widely varying temporal and spatial scales

- Methods to deal with uncertainties including propagation of errors in data and in models

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Science Modeling & Computation for AFCI

Grand Challenge

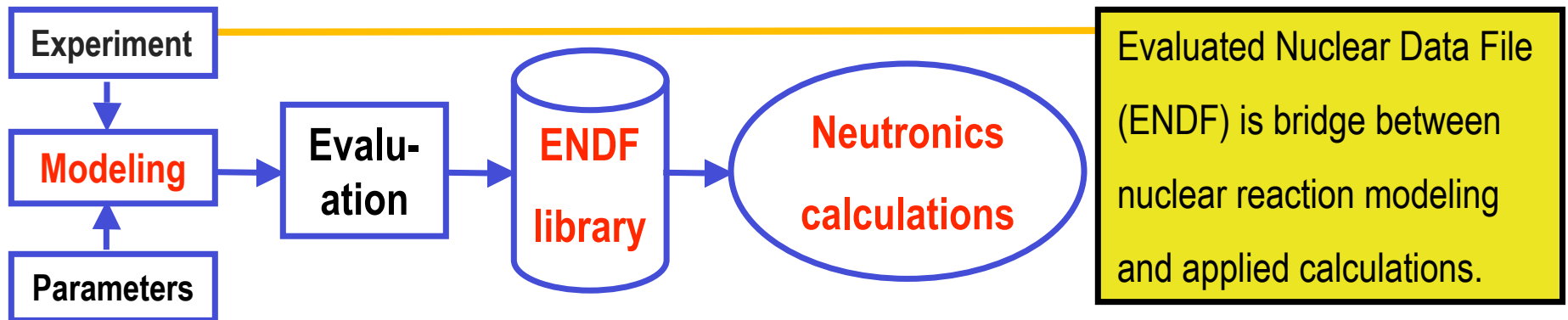## Nuclear Data (5-10 years)

- **Nuclear data covariances**
  - Important for quantification of margins & uncertainties in reactor design (criticality, transmutation, ...), reduction of cost
  - Strong request from AFCI and other user communities
  - New methods must be developed, covariances produced

- **Precise actinide cross sections**
  - Important for AFCI neutronics calculations (k-eff)
  - Major actinides (239-Pu and 235,238-U → capture)
  - Minor actinides (Np, Am, Cm →fission, capture)

Nuclear Modeling

Experiment → Modeling ↔ Parameters → Evaluation → ENDF library → Neutronics calculations

Evaluated Nuclear Data File (ENDF) is bridge between nuclear reaction modeling and applied calculations.

- **Nuclear modeling** is traditionally closely linked to nuclear technology applications

- Nuclear **reaction theory** provides theoretical basis and tool for nuclear data evaluation → **Evaluated Nuclear Data File (ENDF)**

- ENDF database serves as **input** for neutronics calculations and transport codes

- There is **well established mechanism** to maintain ENDF database, synergy of:
    - Cross Section Evaluation Working Group (~15 laboratories, ~50 scientists, supported mostly by DOE-NNSA, partly by **DOE-SC**)
    - US Nuclear Data Program (~ 40 scientists, supported by **DOE-SC**)
    - National Nuclear Data Center, BNL (supported by **DOE-SC**)

Precise Cross Sections for Actinides

Cross sections needed for

- Simulation of **nuclear criticality** and **transmutation rates (burnup)**
- Simulation of **radiation damage** and **heating**

Minor actinides

- **Np, Am, Cm** isotopes
- **Experiments** with extremely small radioactive targets at LANSCE
- **Theory** can be used to predict unknown actinide fission and capture
- **Integral validation** provides very accurate quality check

Major actinides

- ^{239}**Pu,** ^{235,238}**U** have **high impact** on AFCI because of their abundance
- Significant uncertainties (> 10%) in **fast neutron region** for capture
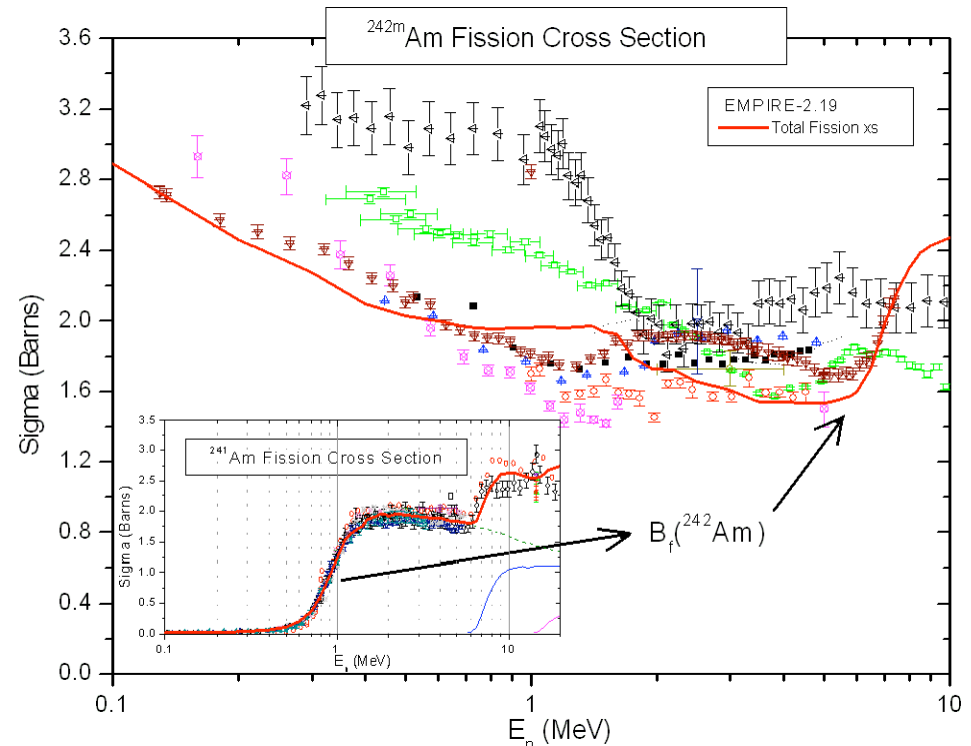
^{242m}**Am fission cross sections current status**

Objectives for AFCI project

- Perform **experiments**
- Improve **modeling**
- Produce precise **cross sections**

Uncertainties & Covariances

What is covariance matrix?

- It is a matrix that specifies the **numerical uncertainties** for a particular data set.

Strong customer demand!

- **Advanced reactor** programs
- **Stockpile stewardship (QMU)**
- **Criticality safety, …**
  - Information needed for **Safety**, **Cost**, and **Quality Assurance**

ENDF/B-VII covariances

- Covariances now exist for only a **very few isotopes** in (not yet released) ENDF/B-VII library
- Most are **poor quality** and **incomplete**
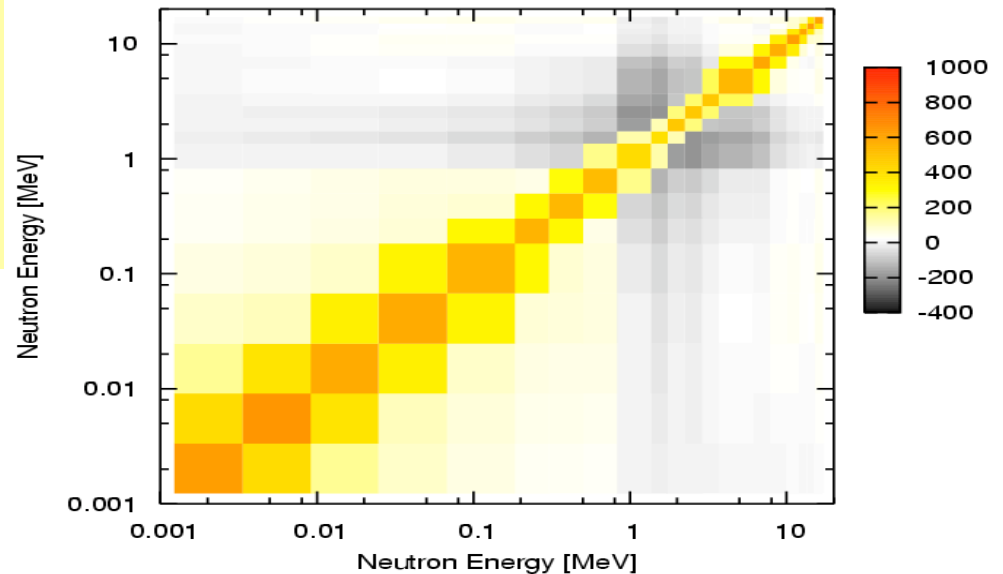
Graphical pattern of typical covariance correlations

Objectives for AFCI project

- Develop **new methods** & **codes, based on Bayesian methods** and **advanced nuclear theory simulations**
- Prepare **covariance** files for **ENDF/B-VII upgrades**

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Impact of cross section uncertainties on reactor design

Example 1:
Accelerator- driven ADS design

- Uncertainties in cross sections for Np, Cm, Am isotopes led to **significant differences in predicted criticality**.

- Need to determine cross sections more precisely.

- Need to quantify uncertainties (**covariances**).

- Similar sensitivities have been determined recently by Palmiotti (ANL).

Comparison of **burn-up reactivity** change
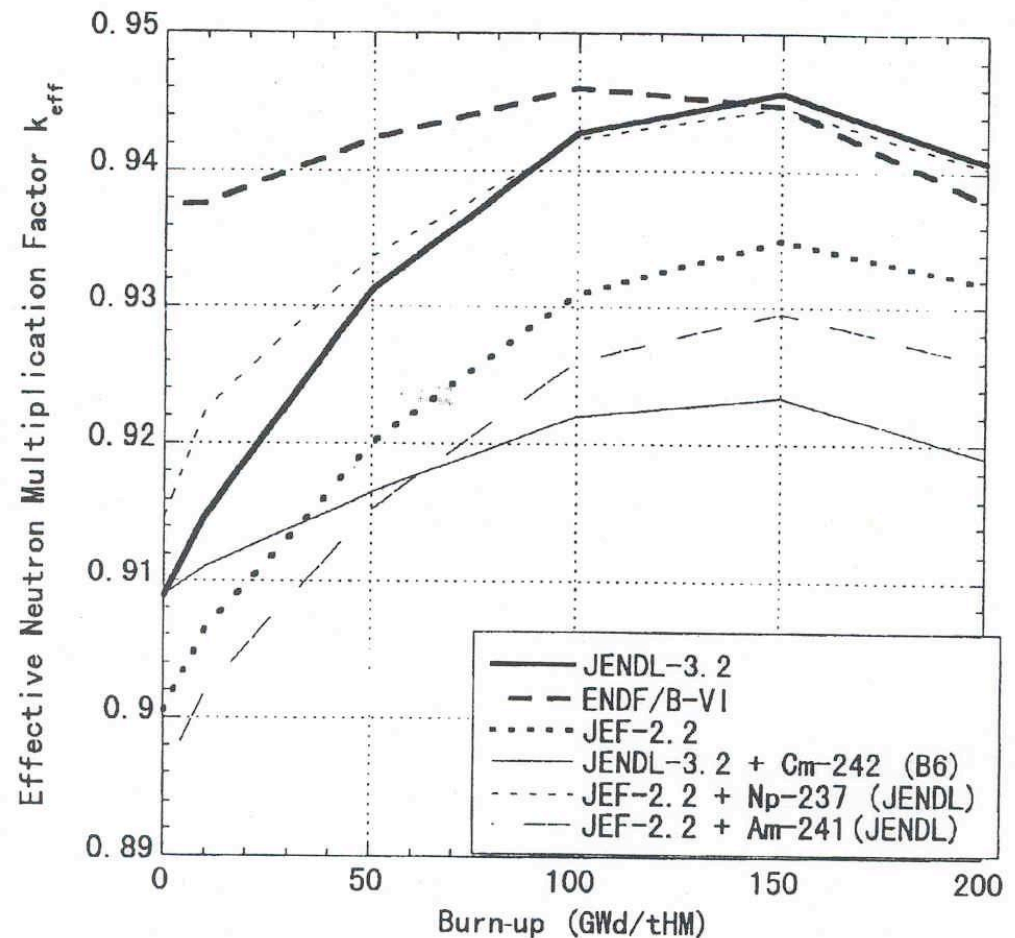
Source: Nuclear Energy Agency (NEA) Working Group on Evaluation Cooperation

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Impact of cross section uncertainties on reactor design

Example 2: Fast Reactor Design (sodium-cooled MOX)

Ishikawa at **ND2004** Nuclear Data Conference, Santa Fe (ed. Haight, Chadwick et al; sponsored by DOE/Science)

Studied impact on **criticality** and **burn-up** (transmutations)

Conclusions:
- **Covariance data** must be included in ENDF etc database
- ^{238}U, ^{239}Pu capture, inelastic & fission must be better determined
- **Minor actinides** Np, Am, Cm and **fission product** improvements needed

"Recently in Japan, it was recognized that nuclear data **covariances are indispensable** to rationally evaluate predicted accuracy of reactor core parameters."

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